

(O,1,1,1,2,3,3,3-2H8)Propan-2-ol  
22739-76-0 | DTXSID30177279

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $5.72 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $7.36 \times 10^{-1}$

**Confidence level:**  $6.66 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Isopropanol

**Measured:**  $5.07 \times 10^{-12}$

**Predicted:**  $5.72 \times 10^{-12}$

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1-Propanol

**Measured:**  $5.53 \times 10^{-12}$

**Predicted:**  $7.35 \times 10^{-12}$

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1,4-Diazabicyclo[2.2.2]octane

**Measured:**  $2.20 \times 10^{-11}$

**Predicted:**  $1.30 \times 10^{-11}$

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Diethyl ether

**Measured:**  $1.31 \times 10^{-11}$

**Predicted:**  $9.74 \times 10^{-12}$

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tert-Butyl alcohol

**Measured:**  $1.12 \times 10^{-12}$

**Predicted:**  $3.20 \times 10^{-12}$